Modeling chemistry in protoplanetary disks

Karen Willacy
Geoff Bryden
Bill Langer

JPL

Outline

- Two models
  - Deuterium chemistry

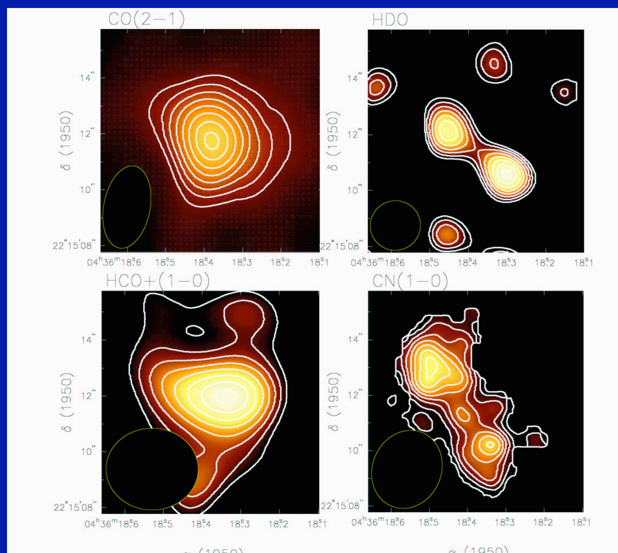
    Important to trace the thermal history of the disk and interstellar/disk links
  - Vertical mixing

    Can turbulent mixing in the vertical direction affect column densities in the disk

Observations of disks

- Mostly sensitive to outer disk (> 50 AU)
- Trace region with T = 20 - 40 K and n = 10^6 - 10^8 cm^{-3}
- Fractional abundances are lower than in molecular clouds (factor of 10 - 100).
- Important processes
  - Ion-molecule e.g. HCO^+
  - Photoprocesses e.g. CN/HCN ratio
  - High deuteration ratios
  - Low abundances of complex species e.g. H_2CO, CH_3OH

LkCa15



T Tauri star

Distance = 140pc

Dust mass = 10^{-4} - 0.2 $M_{\odot}$

Age = 3 - 5 Myrs

Radius = 600 AU

Kessler 2003

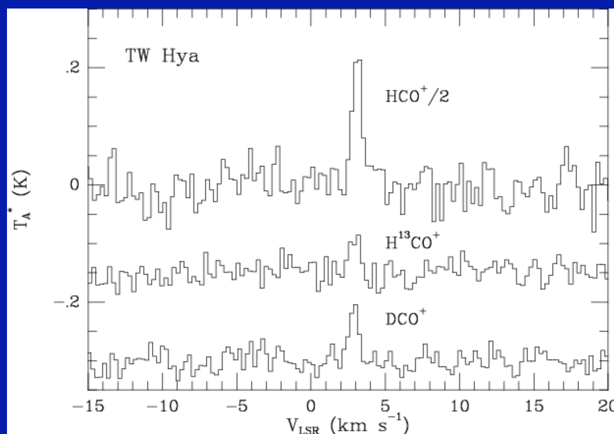
OVRO observations of LkCa15

HCN - traces outer region with dip in column density in the center

CN - indicates photodissociation processes

HCO+ - indicates ion-molecule reactions - central peak

TW Hya



T Tauri

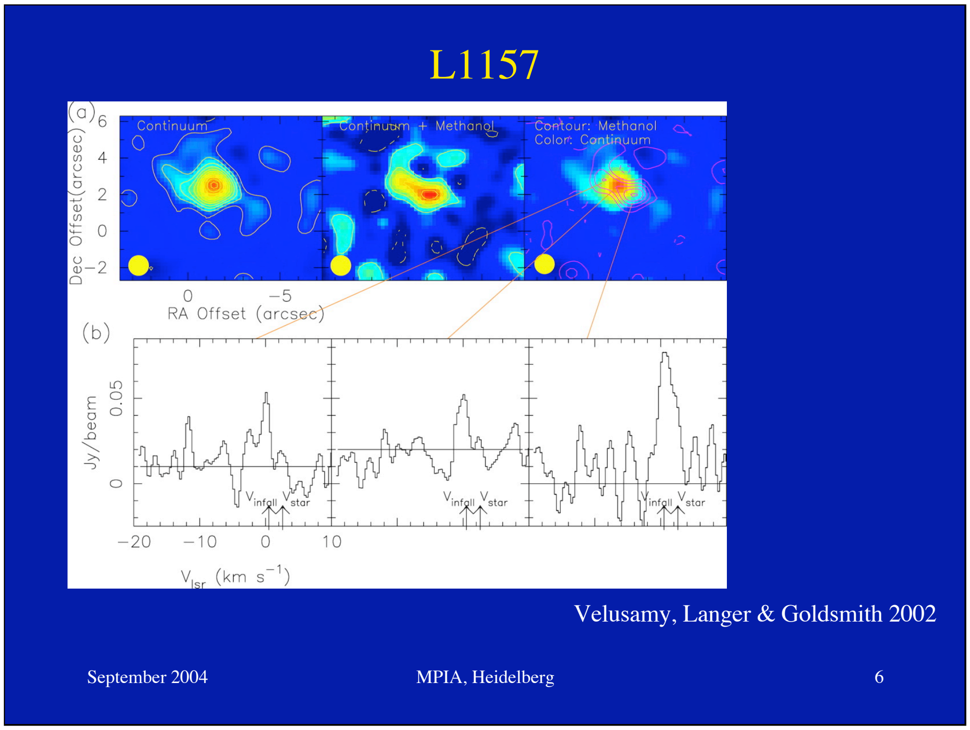
Distance = 56pc

Age = 8 Myrs

Radius = 800 AU

Dust mass = 2 x10^{-2} $M_\odot$

Van Dishoeck et al. (2003)



Maps of dust continuum and methanol spectral line emission at 1mm from disk in L1157

Color image - continuum

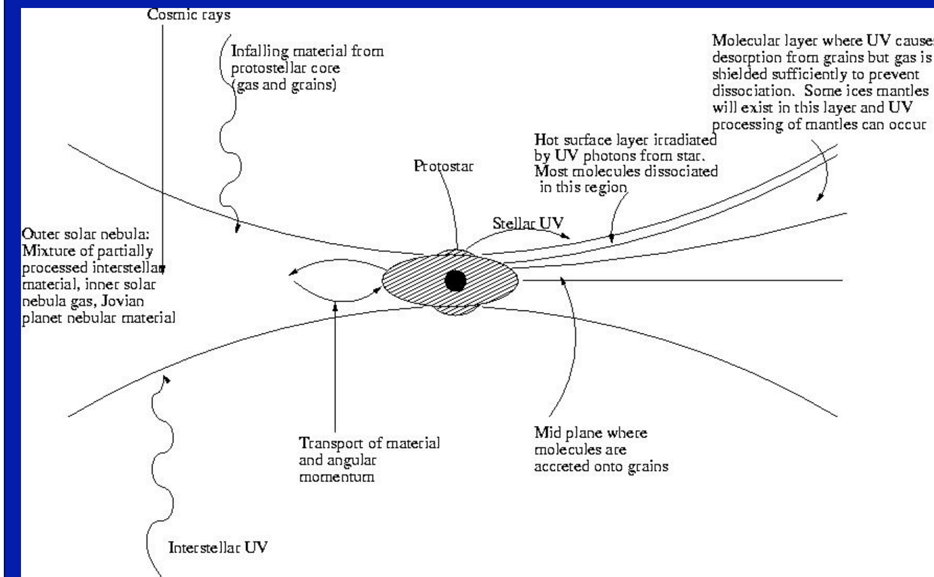
Line = CH3OH

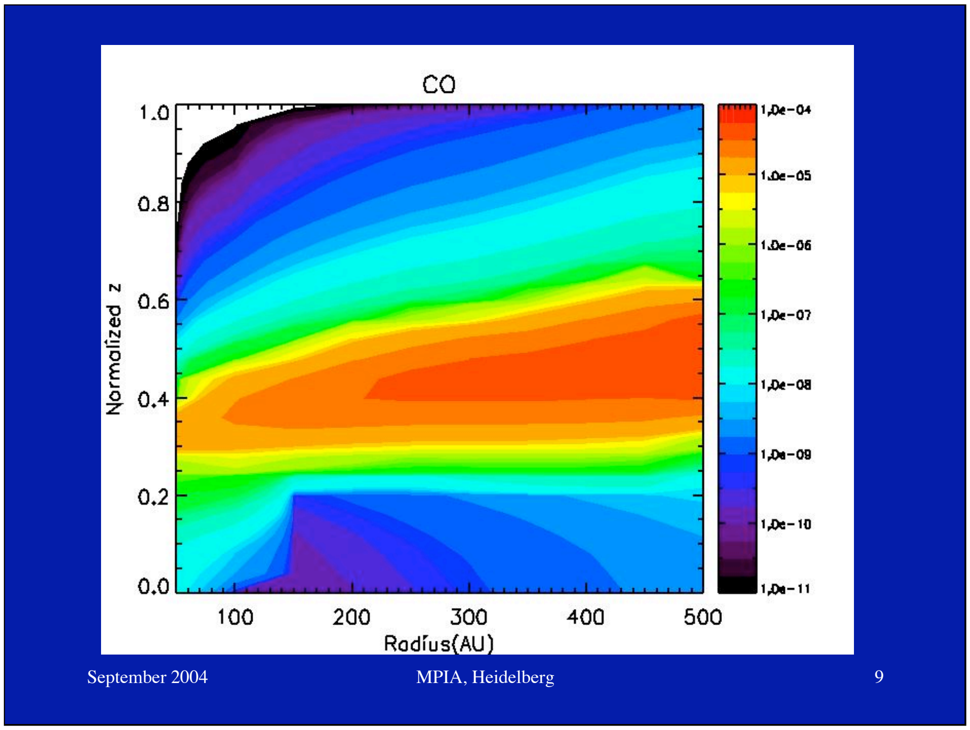
Structre and kinematics of methanol emission indicate that the gas is tracing a warm layer in the infall-disk interface, consistent with an accretion shock,

Previous flared disk models

- Aikawa et al. (1999, 2001)
  - Kyoto minimum solar mass nebula model
  - Low temperature, isothermal model, requires low sticking coefficient (S_x = 0.03) to maintain gas phase molecules
- Willacy & Langer (2000)
  - Chiang & Goldreich (1997) 2 layer model
  - Require efficient desorption process to keep molecules in the gas (photodesorption)
- Aikawa et al. (2002), van Zadelhoff et al. (2003)
  - D'Alessio et al. (1999) models with continuous vertical T gradient
  - Disk is warm enough that thermal desorption is efficient and can produce high abundances of molecules in the gas even for S_x = 1

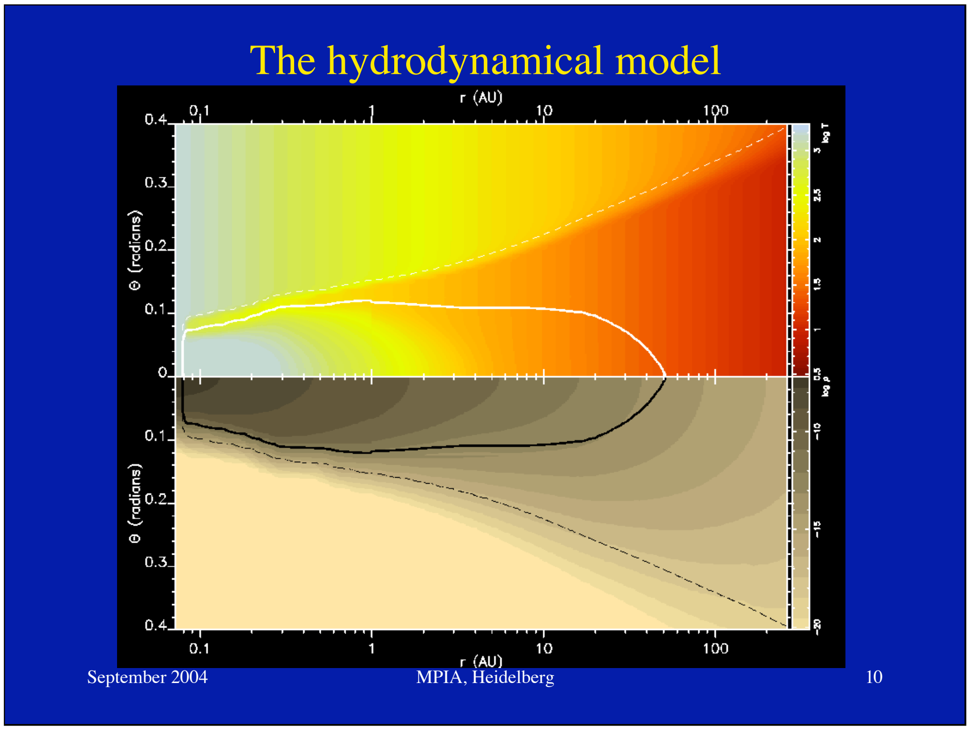
Chemical structure of disks





Fractional abundance of CO in disk

Shows 3 layer structure, with CO molecule existing in band, above the mid-plane and below the UV irradiated surface layer



Bryden et al.

Describes a geometrically thin disk

Heated viscously and by radiation from central star

Temperature is calculated self-consistently

Assumes disk is in steady state I.e. disk properties are independent of time and mass accretion rate is constant

Structure of disk is determined by solving hydrodynamic equations in a semi-analytic fashion

Mass accretion rate = 1e-8 solar masses per year

Surface density = 1000 g cm-2 at 100AU

Surface density = sigma_0 R^(-3/2) R> 16 AU

Surface temperature proportional to R^(-3/7)

Top half of plot is temperature - shows heated surface layer

Bottom half is density

Solid dark line is surface of disk based on vertical depth of its own infrared radiation

Dotted line is optical surface to radial visible stellar radiation

Disk is stable if

H/r > M_disk/M_star

The chemical model

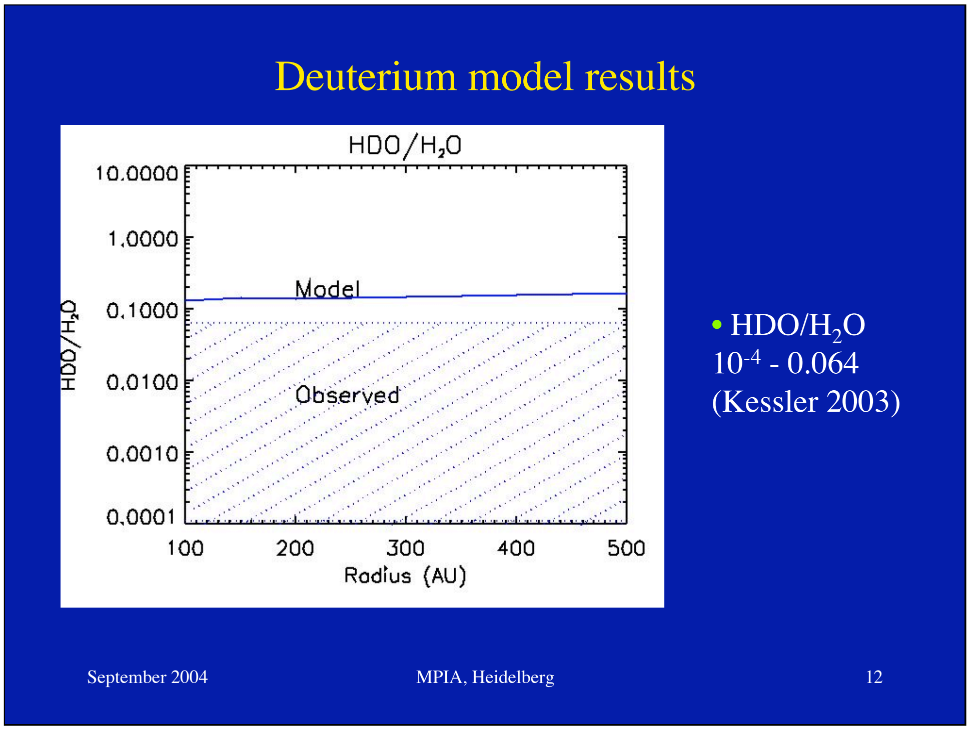
- Based on Millar et al. (1997) (UMIST ratefile)
- 268 species (gas and grain), 5312 reactions
- Include thermal desorption, cosmic ray heating and photodesorption
- Deuterium reactions (based on Willacy & Millar 1998, Rodgers & Millar 1996)
- Include H_2 and CO self-shielding using method of Lee et al. (1996).
- Photodissociation by both interstellar and stellar UV photons
- Input abundances from the output of a molecular cloud model at 1Myrs

Desorption processes -

Thermal - material desorbs as temperature reaches its sublimation temperature so strongly bound molecules desorb at higher temperatures

Cosmic ray heating - not efficient enough for most molecules to make a difference

Photodesorption - included to represent some kind of efficient desorption, the cooler temperatures in our model which arise from the use of a more realistic grain size distribution (instead of an interstellar distribution) means that thermal desorption is not sufficient on its own to maintain observable gas phase column densities of many species. Photodesorption is potentially very efficient if the lab work of Westley et al. (1995) is correct but we use it here mainly as a representative desorption process rather than claiming that the extra desorption process has to be photodesorption (desorption processes are a matter of contention!).



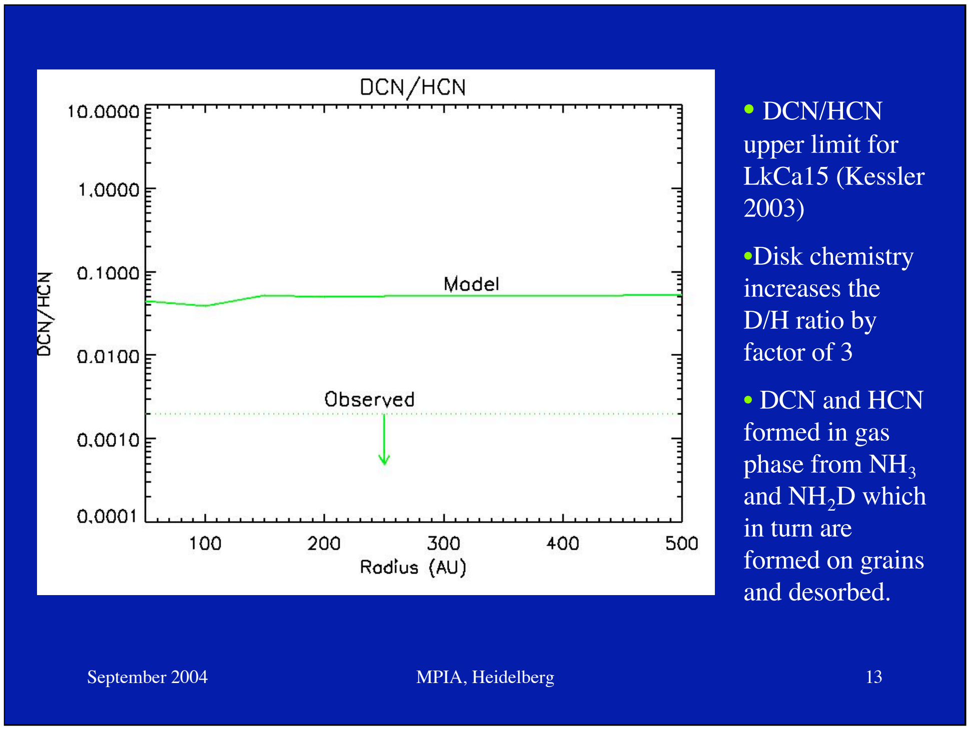
General comments - compared to observations of DM Tau, LkCa15, TW Hya

Differences in physical parameters of model compared to sources could affect the comparison e.g.disk mass - higher disk masses could result in higher column densities. But in general we find fairly good agreement with many molecules agreeing with observations to a factor of a few. Given uncertainties in the models this is good to see!

Upper limit observed = 0.0001 - 0.064

Model ~ 0.2

HDO/H2O is determined by grain chemistry and desorption.



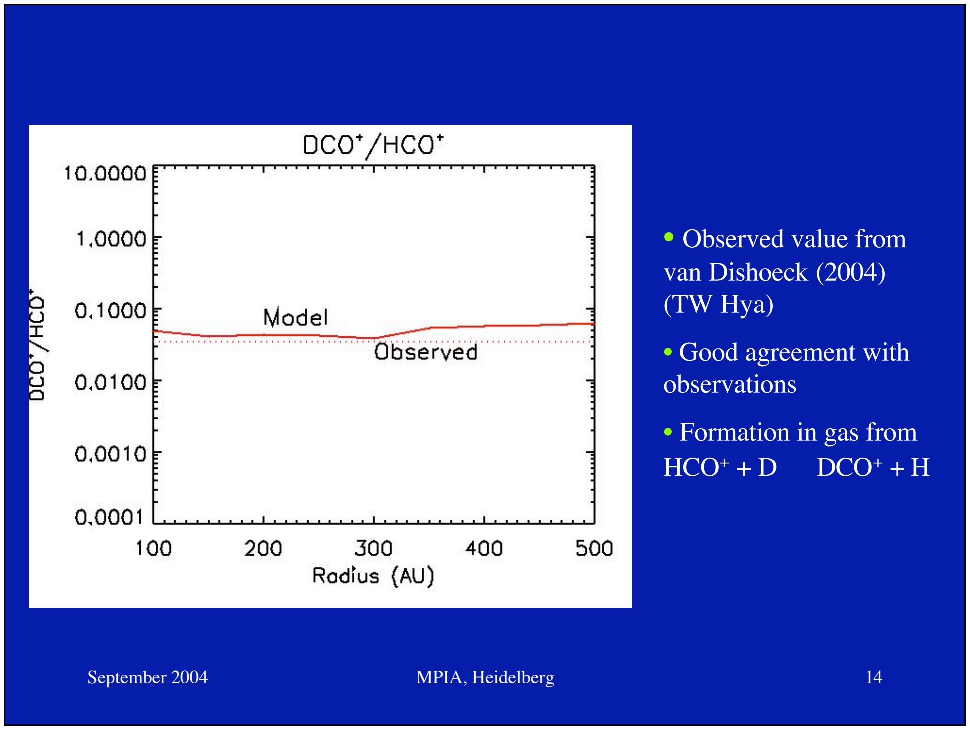
Observed value in disk is less than the observed value in TMC-1 (value = 0.023).

Model input value is 0.014 close to TMC-1 value.

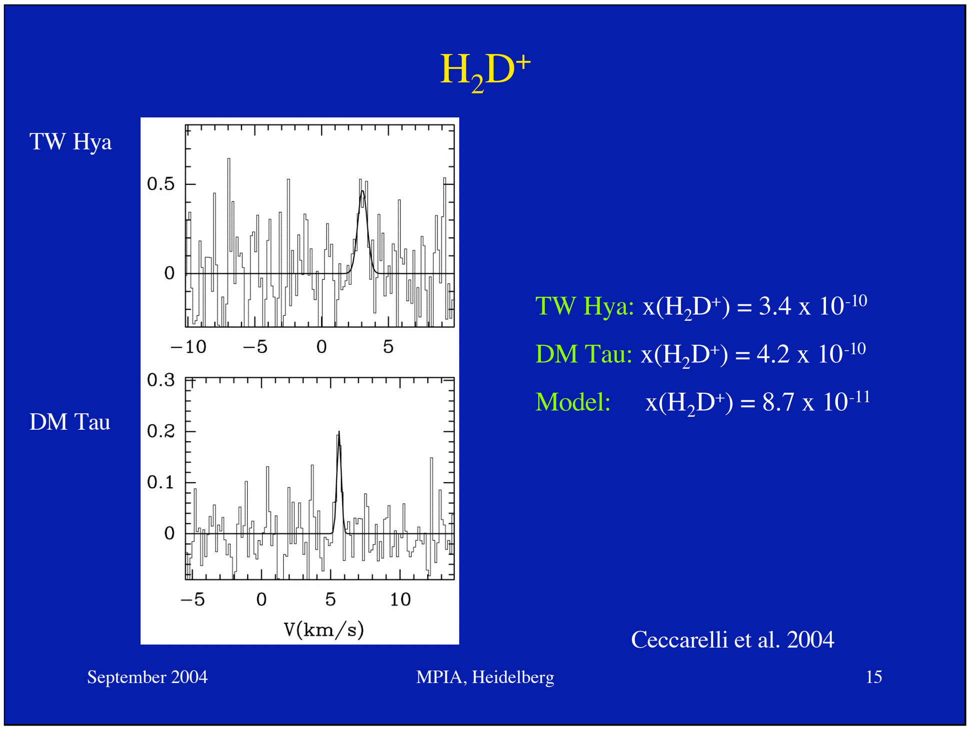
Model increases ratio, but observations suggest that the ratio is decreased in disks

DCN/HCN ratio therefore reflects the grain D/H abundance of NH2D/NH3

May indicate that the grain chemistry formation of Nh3 etc is too efficient



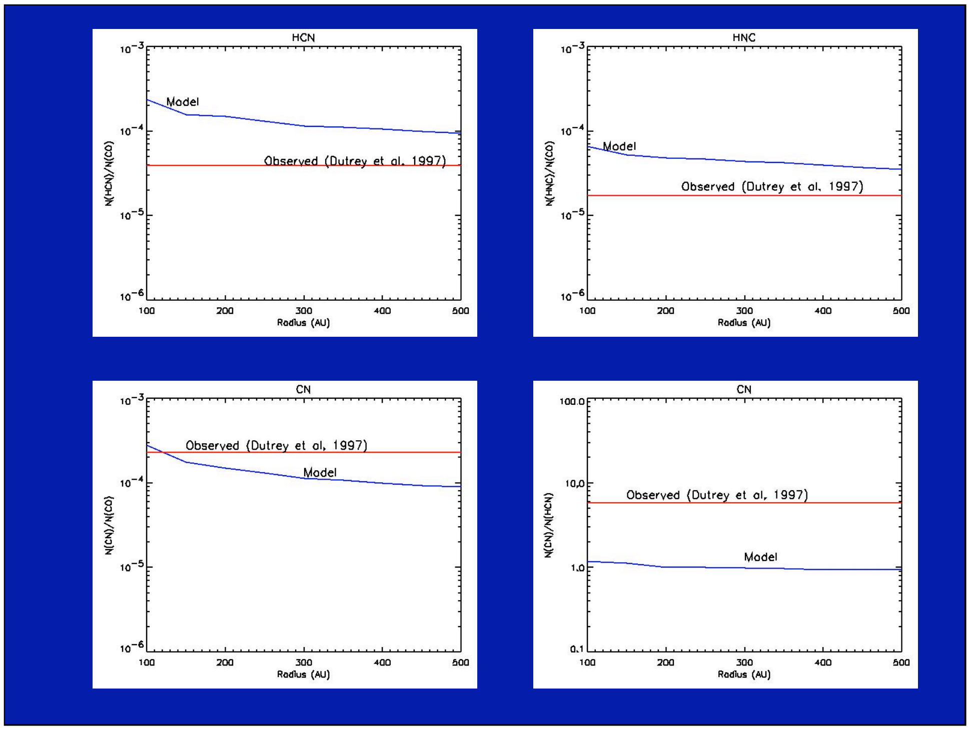
Ratio determined by abundance of atomic D.



Observations thought to trace the midplane where the gas is cold and depleted of CO.

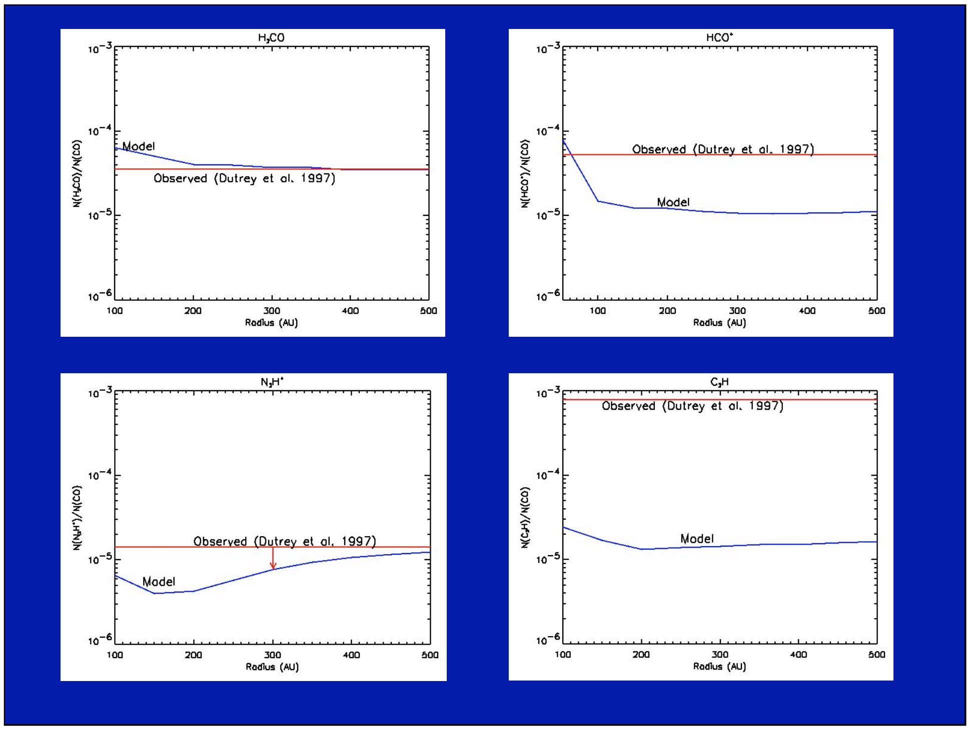
Model value is for 300AU at midplane.

Agreement within a factor of 5 - pretty good!



Good agreement (within a factor of a few) for many molecules in outer disk

CN/HCN a bit on the low side - could be due to low stellar UV field, or to the lack of proper treatment of the radiative transfer



Good agreement in outer disk except for C2H - again photodissociation product, could be problems with radiative transfer or the low UV field from the star.

Results

- Successes -
  - Good agreement with many observed abundances including the D/H ratios for HCO^+ and H_2O

- Problems
  - Can't account for the observed abundances of molecules such as C_2H and CN which are formed by photodissociation. Need a better description of the radiative transfer in the disk

Diffusion model

- Disks are turbulent
  - Efficient angular momentum transport required
  - Physical conditions in disks turbulent transport only process that can achieve this transport
- Shakura & Sunyaev (1973)
  - Introduced an ‘anomalous’ viscosity component proportional to gas pressure
- Lyndon & Pringle (1974)
  - $_t =$ c_s h

Efficient angular momentum transport required - molecular viscosity is not efficient enough. Therefore turbulence was invoked. Source of this turbulence is still uncertain, could be MHD, hydrodynamical or gravitational.

Pringle - from this can construct models of vertically averaged alpha disks.

V_t = turbulent viscosity

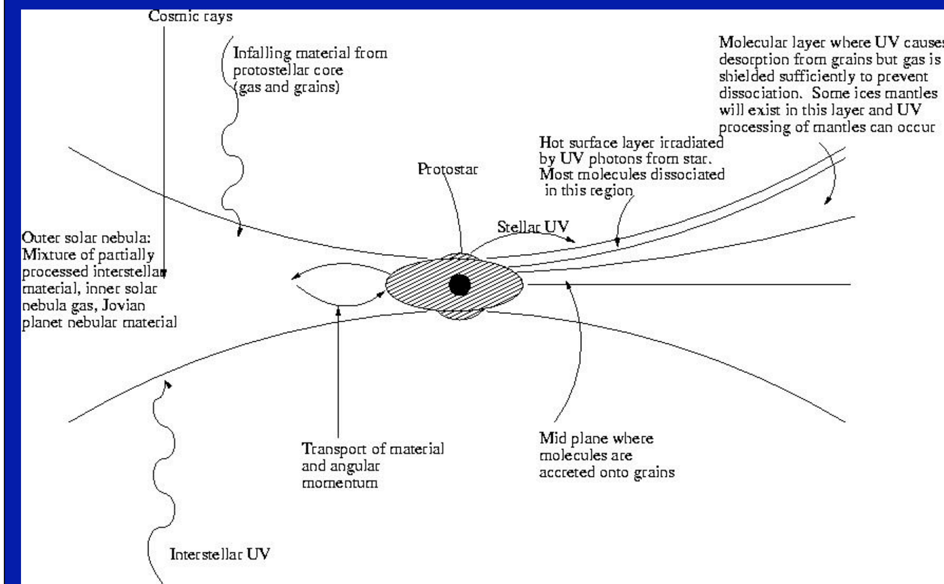
Alpha = dimensionless parameter < 1

C_s = sound speed

H = disk height

From this models of vertically average alpha disks can be constructed.

Why diffusion might affect chemistry



- Code originally used for atmospheric chemical models (Allen, Yung & Waters 1981, Shia et al. 1990), and for modeling molecular clouds (Xie, Allen & Langer 1995, Willacy, Langer & Allen 2002)
- Uses mixing length theory
- Assumes diffusion timescale for given tracer depends on its composition gradient

Mixing length theory - characterises turbulence as eddies that maintain different properties to the average fluid in which they exist for the time taken to travel a distance l - the mixing length

Eddies remain separate to the ambient fluid for long enough to travel a distance l - the mixing length

1-D diffusion

Fluctuations in fractional abundance x_i due to turbulence can be parameterized as

$$x_i = \quad l \frac{dx_i}{dz}$$

Net transport flux:

$$_i = n(H_2) \langle v_t \quad x_i \rangle = \quad Kn(H_2) \frac{dx_i}{dz}$$

$$_i = \quad Kn_i \quad \frac{1}{n_i} \frac{dn_i}{dz} \quad \frac{1}{n(H_2)} \frac{dn(H_2)}{dz}$$

K = diffusion coefficient = $\langle v_t l \rangle$

Dx_I/dz = abundance gradient in the z direction, l = mixing length

V_t = turbulent viscosity

- Chemical continuity equations

$$\frac{\partial n_i}{\partial t} + \frac{\partial \Phi_i}{\partial z} = P_i - L_i$$

- Turbulent code solves coupled continuity equations using finite differencing method
- Code allows different temperatures, densities, diffusion and advection coefficients in each zone

P, L = production and loss terms of species I

Phi_I = net transport flux

Estimating K

- Estimate diffusion coefficient K by

$$= {}_t$$

$$_t = c_s h$$

For 100 AU
  = 0.001,
h = 0.09 x 100 AU = 1.35 x 10^{14} cm
c_s = 4.4 x 10^{3} cms^{-1}
K = 6 x 10^{15} cm^{2}s^{-1}

- We use K between 10^{18} and 10^{20} cm^{2}s^{-1}
- We assume K constant with R and z

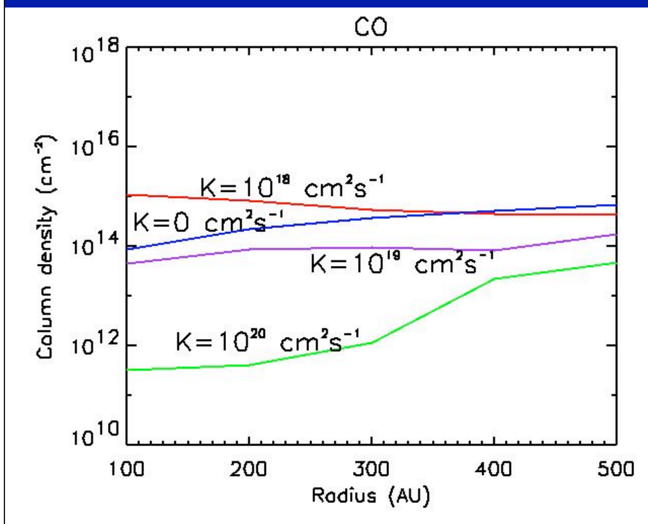
September 2004 MPIA, Heidelberg 24

C_s = sound speed

H = scale height

Alpha = alpha parameter used to describe viscosity in disks

Computational problems with K < 1e18



•K=0 and K = 10^{18} cm^2s^{-1} models:

- CO cycles between gas and ice phases by freezeout and cosmic ray heating
- With diffusion, ice coated grains move upwards in disk to heated region increasing N(CO) due to thermal desorption

•K > 10^{18} cm^2s^{-1} models:

$$CO_{gr} \rightarrow CO_{gas} \xrightarrow{h\nu} C + O$$

$$C \xrightarrow{h\nu} C^{+} \xrightarrow{H_2} CH_2^{+}$$

September 2004 MPIA, Heidelberg 25

Low levels of diffusion increase column density at small radii, but higher values actually decrease it.

AT 200 AU and 1Myrs:

CO ice forms in midplane. In K=0 model, it is desorbed by CR heating and cycles between gas and grain phases.

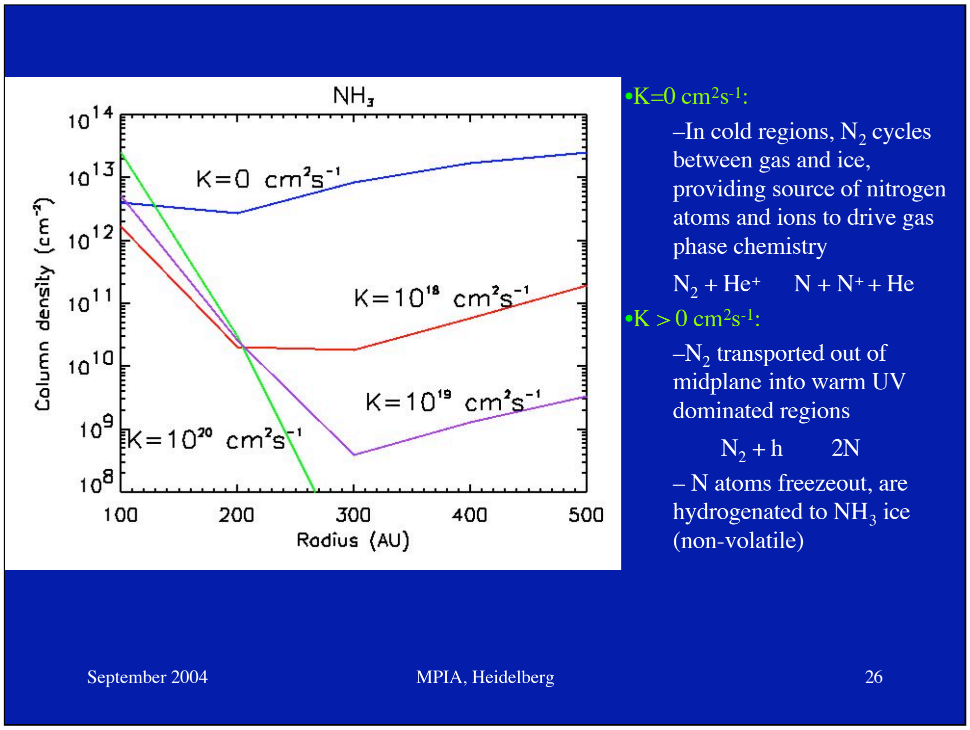
In K=1e18 model, ice coated grains transported out, CO desorbed thermally, cycles between gas and grain - get ice and gas at higher z than in K=0 model

For higher values of K

Ice coated grains transported outwards, CO desorbed, but in outer layers it is also photodissociated into C and O. C is photoionized to C+, which reacts with H2 to start chain that forms CH4. Therefore CO is gradually changed into CH4. For K=1e20 model, CH4 ~ 5x higher in midplane than x(CH4) in K=1e18 model and extends to higher z.

Low K - thermal desorption in upper layers balances accretion in lower layers so CO abundance in gas remains high. Little processing into other molecules

High K - CO dissociated in upper layers, converted into carbon atoms and then into hydrocarbons such as methane



Diffusion reduces column densities at all values of K

All nitrogen bearing molecules show reduced column densities with the addition of diffusion for R > 150 AU.

In K=0 model, NH3 is present in the midplane region z< 1.4e15 cm

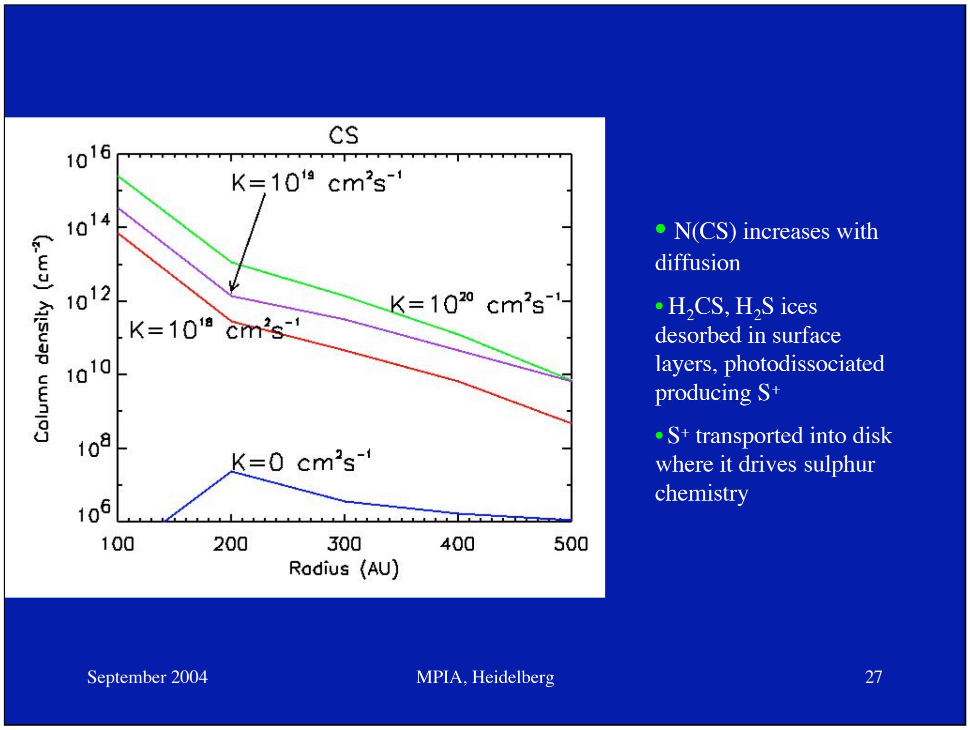
It forms from desorption of N2 from grains, which reacts with He+, producing N and N+ which drive N chem

In outer region, N2 desorbs, is photodissociated into 2 N atoms, which then freezeout and form NH3 on grains, without much being left in gas therefore little gas phase chemistry. N ends up in NH3 ice which is non-volatile and remains on grains (photodesorption not included here).

So in K>0 models, N2 processed into NH3 ice in outer regions, transported into lower levels where it can't be desorbed and there is no resevoir of Natoms for gas phase chemistry. Therefore N ends up trapped on grains in NH3 ice and N(NH3) gas phase column density falls.

At small radii:

NH3 forms on grains in cold mid-plane. Diffusion moves the grains into warm region where NH3 is desorbed thermally. Hence there is a warm layer containing high abundances of NH3 in the gas. Increasing K increases the movement of NH3 ice from the midplane upwards



Column densities of CS are increased with diffusion.

Dissociation of sulphur molecules in upper layers (e.g. H2CS, H2S which are partially desorbed - thermally, BE = 2000K for H2S and 2250K for H2CS so there is some desorption in warm surface layers). This provides source of sulphur atoms.

Diffusion allows S+ to be transported into disk where it can drive a sulphur chemistry, resulting in an increase in the CS abundance in the molecular layer.

Increasing K increases the thickness of the layer that contains S+ and therefore sulphur molecules, so sulphur molecules are present deeper into the disk.

Conclusions

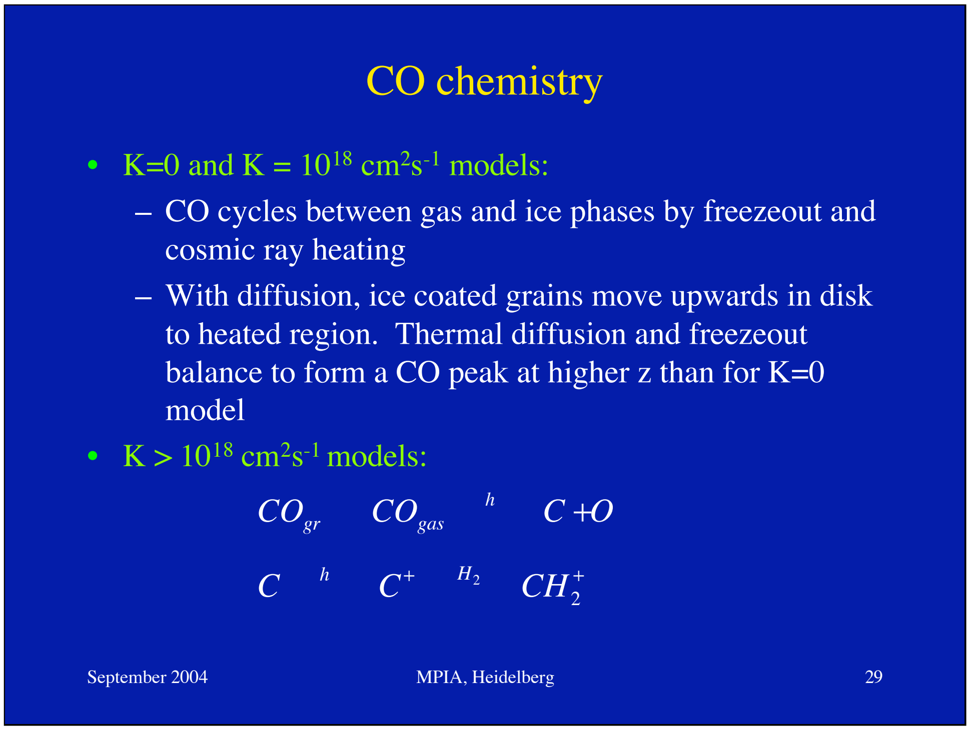
Mixing model:

- Mixing can greatly affect the abundances
- Effects of mixing are molecule dependent.

Deuterium model:

- Good agreement with observations for many molecules in outer disk
- Good agreement for D/H ratios of H_2O and HCO^+
- Good agreement with midplane abundance of H_2D^+
- Some problems with photodissociation products - need better description of radiative transfer

Some molecules show increase in column density, others are decreased, mixing greatly complicates the chemical processing.



Low K - thermal desorption in upper layers balances accretion in lower layers so CO abundance in gas remains high. Little processing into other molecules

High K - CO dissociated in upper layers, converted into carbon atoms and then into hydrocarbons such as methane

Observations

- Use observations of LkCa15 (Kessler 2003, Qi 2001), DM Tau (Dutrey et al. 1997) and TW Hya (van Dishoeck et al. 2004).
- Observations from outer disk
- LkCa15: Dust mass = 0.2 $M_{\odot}$, age = 3-5 Myrs,
  radius = 600AU
- DM Tau: Mass = 0.03

Observations from outer disk - R > ~ 100 AU

Therefore some differences between model and observations would be expected because of different physical parameters - future models will consider specific sources.

Aikawa & Herbst 2001 - found that higher disk masses lead to higher D/H ratios